MPA materials matter

May 2008

Newsletter of the Materials Physics and Applications Division

DOE honors Center for Integrated Nanotechnologies

CINT Gateway to Los Alamos

Department of Energy Secretary Samuel Bodman honored the LANL/SNL Center for Integrated Nanotechnologies (CINT) for effective management of construction and instrumentation projects at CINT's Gateway to Los Alamos facility and Albuquerque's Core facility. Bodman presented the Award of Achievement at the bi-annual DOE Project Management Workshop in Washington, D.C. The nanotechnology center was one of two DOE engineering construction projects receiving recognition.

The integrated LANL/SNL project team credited extensive communication and planning for the team's ability to respond to unanticipated challenges arising during the construction period, such as the Laboratory-wide "stand down," a continuing resolution affecting the federal budget, and escalating costs for materials and labor. The Gateway and the Core facilities were completed in April 2007 at a cost of $75 million, although basic operations began in 2006. Both facilities comprise more than 130,000 square feet of space. LANL's CINT includes laboratories to house cutting-edge technologies, including ultrafast spectroscopy, self-assembly, physical synthesis, scanning probes, pulsed laser deposition, and a visualization theater.

A joint LANL/SNL team, led by LANL Director Toni Taylor and Sandia Co-Director Robert Q. Hwang, manage CINT. Established as a national user facility,

From left to right: Neal Shinn, SNL, CINT project leader; Alex Lacerda, interim MPA division leader; Bill Hendricks, SNL, CINT project leader, Core facility; Will Ortiz, overall DOE project manager, Albuquerque site office.

CINT is devoted to establishing the scientific principles that govern the design, performance and integration of nanoscale materials. LANL/SNL CINT is one of five DOE Nanoscale Science Research Centers (NSRCs), premier national user facilities for interdisciplinary research at the nanoscale. NSRCs are a suite of complementary facilities providing researchers with state-of-the-art capabilities to fabricate, process, characterize, and model nanoscale materials, and constitute the largest infrastructure investment of the National Nanotechnology Initiative.

CINT Core facility at Albuquerque

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From Alex's desk

Materials Physics and Applications: Strategic planning

Since mid-October 2007 MPA-DO has been working with your local leadership to define the Division's short- and long-term strategic plans. I find this to be an important exercise, which indeed cannot be accomplished only by memos and just your local leadership. For our strategic plan to succeed you all have to be involved, interested, and a part of it. As a Laboratory we are doing better as far as defining our strategic plan, but we still have a ways to go, particularly in regards to getting our technical staff involved and a part of the process. MPA's strategic plan will be along the Institution's capability model.

And speaking about capability, the 2008 Materials Capability Review went really well and the Institution received good feedback. I have distributed a copy of the first draft of the committee's report to your groups/center leaders and I encourage you to take a look if you are interested. MPA's strategic plan will not only be based on our current strengths, but also in areas we believe we are able to expand. Our strategic plan has a direct connection to our capabilities of delivering materials solutions to national needs. We have identified the following set of capabilities with the respective leaders: Functional materials: synthesis and processing (Leader: Kevin Ott, MPA-MC); Materials under extremes (Leader: Marcelo Jaime, MPA-NHMFL); Translating science to solutions (Leader: Cathy Padro, MPA-11); Fundamental properties of materials (Leader: Mike Hundley, MPA-10); Novel experimental tools (Leader: Toni Taylor, MPA-CINT); and Partnership/collaborations (Leader: Ken Marken, MPA-STC).

By the beginning of June, I would like to see a small team be identified by the respective capability leaders where the following topics will be addressed: funding (current and opportunities), key personnel (current and possible strategic hires), capability elements (facilities, tools, and opportunities to expand), and finally, issues. Your participation is of paramount importance. I hope you will be hearing from your local leadership soon and start getting engaged.

Congratulations

Two MPA postdoctoral researchers are recipients of Los Alamos Postdoctoral Distinguished Performance Awards.

Ki-Yong Kim (MPA-CINT) is recognized for major accomplishments in the development of ultrafast terahertz (THz) radiation as a diagnostic to study and characterize fundamental properties of materials, dense plasmas, and electron bunches in synchrotrons, free electron lasers, and intense laser-based electron accelerators.

Pinaki Sengupta's (MPA-NHMFL and T-11) theoretical works have significantly contributed to the quantitative microscopic understanding of physics of quantum magnets and established connections to other seemingly distinct collective phenomena in condensed matter.

Sengupta also recently received honorable mention in the Leon Heller Postdoctoral Publication Prize in Theoretical Physics for his for his paper, "Field-Induced Supersolid Phase in Spin-One Heisenberg Models" published in *Physical Review Letters* in June 2007 and co-authored with Cristian Batista, T-11.

Please join me in congratulating Cathy Padro as MPA-11 permanent group leader. Cathy joined the Laboratory in 2003 as project leader for hydrogen and biomass systems. Cathy is the Laboratory lead for the DOE's safety, codes and standards activities in the DOE/EERE Hydrogen, Fuel Cells and Infrastructure Technologies Program, focusing on the development of performance-based codes, standards, and regulations for hydrogen applications, hydrogen safety sensors, and fuel quality standards. She participated in the 2005 Director's Development Program and served as the MPA deputy division leader for four months. Cathy is a licensed chemical engineer, with bachelor's and master's degrees from State University of New York at Buffalo, and has more than 25 years of experience in the design and analysis of conventional and alternative energy systems.

Prior to 2003, she was the hydrogen technology manager at the National Renewable Energy Laboratory in Golden, Colorado. There, she led scenario planning and road-mapping efforts for the DOE hydrogen program, including assisting its advisory panel in the development of long-range scenarios for hydrogen energy systems.

Dean Peterson is stepping down as MPA-STC Center Leader, returning to research after playing a pivotal role in creating new industrial partners and advancing the center's capabilities since 1992.

Dean, who earned his PhD in physical chemistry from the University of Kansas, joined Los Alamos in 1972 as a troubleshooter in CMB-5 developing nuclear heat sources for interplanetary missions such as Pioneer, Viking, Galileo, and Voyager.

Prior to the creation of the Superconductivity Technology Center, he served as high temperature superconductor (HTS) team leader in MST-5, synthesizing and characterizing phase behavior of high temperature superconductors, and was the principle investigator on CRADAs (Cooperative Research and Development Agreement) with HP/DuPont, GE, American Superconductor and Intermagnetics General.

In 1992 he became Superconductivity Technology Center Leader. As a member of the High Temperature Superconductor Wire Teams, Dean contributed to the development of BSCCO and YBCO HTS tapes in partnership with American Superconductor and Superpower, and provided management for CRADA partnerships and development of coated conductor tapes. He also initiated the carbon nanotube project, which has produced nanotubes with world record lengths and fiber strengths.

MPA-STC in the news

World's first transmission voltage superconductor cable energized in Long Island Power Authority's power grid.

MPA-STC industrial partners, American Superconductor (AMSC) recently announced the successful operation of the superconducting cable project on Long Island, NY at transmission line voltage. The cable utilizes HTS wire produced by AMSC, which also is the prime contractor for the project. The 2,000-foot-long cable system is cryogenically cooled using a liquid nitrogen refrigeration system from Air Liquide. Steve Ashworth, MPA-STC, led a readiness review team that advised on this DOE project on behalf of the Department of Energy and Los Alamos staff made major contributions to AMSC superconductor wire development. This achievement represents another important step towards a national superconducting electric grid based in part on Los Alamos developed technologies.

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Quantum oscillations in the underdoped cuprate $YBa_2Cu_4O_8$

The mechanism for high-temperature superconductivity in the layered copper oxide superconductors has remained elusive for more than 20 years. At the heart of the problem is the evolution of the ground state from a Mott-Hubbard insulator to a superconductor as the number of doped holes *p* per planar CuO_2 unit is increased. In particular, there is no agreement as to how the underdoped region should be described.

Los Alamos researchers and collaborators report the first observation of quantum oscillations in the underdoped cuprate superconductor $YBa_2Cu_4O_8$ using a contactless conductivity (tunnel-diode oscillator) technique in pulsed magnetic fields up to 85T. There is a clear signal, periodic in inverse field, with frequency 660 ± 15T and some evidence for the presence of two components of slightly different frequency. The quasiparticle mass is $m = 3.0 \pm 0.3m_e$. In conjunction with the results of Doiron-Leyraud *et al*. for $YBa_2Cu_3O_{6.5}$, the present measurements suggest that Fermi surface pockets are a general feature of underdoped copper oxide planes and provide information about the doping dependence of the Fermi surface.

The research, "Quantum Oscillations in the Underdoped Cuprate $YBa_2Cu_4O_8$," was published in *Physical Review Letters* **100**, 047003 (2008). Researchers include E. A. Yelland (H.H. Wills Physics Laboratory, United Kingdom); John Singleton, Chuck Mielke, Neil Harrison, and Fedor Balakirev (MPA-NHMFL); B. Dabrowski (Northern Illinois University); and J. R. Cooper (Cambridge).

DOE BES and LDRD support the research. The work at NHMFL is performed under the auspices of the National Science Foundation, DOE, and the State of Florida.

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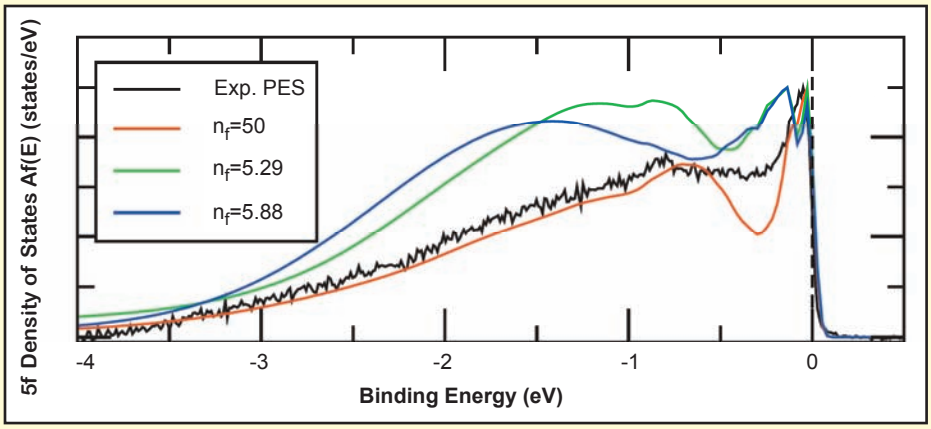
f-electron delocalization in delta-plutonium

Plutonium is probably the most complicated element in the periodic table, based on its condensed matter physics properties, crystal structure, and metallurgy. This behavior is related to its position in the periodic table at the boundary between the light actinides that have itinerant 5f electrons and the heavy actinides with localized 5f electrons. Therefore the plutonium electrons are in a very strongly correlated state. Researchers conducted a systematic analysis of spectral properties of delta-plutonium with varying 5f occupancy by comparing the experimental and theoretical photemission spectra, as shown below. They used dynamic mean field theory (DMFT) to calculate the density of states in the valence band. The results showed the strong sensitivity of spectral properties to 5f occupancy and indicated the "open shell" 5f configuration. This is significant because it defines the degree of f-electron delocalization for delta-plutonium and provides the appropriate computational framework within the dynamic mean field theory approach to examine spectral properties. The researchers demonstrate the need of a rigorous, correlated calculation for plutonium to solve the remaining problems with possible admixture of 5f character in the ground state. The work involved a collaboration of Jian-Xin Zhu and Bob Albers (both in T-11), John Wills (T-01), Tomasz Durakiewicz and John Joyce (both in MPA-10), A. K. McMahan (Lawrence Livermore National Laboratory), and M. D. Jones (SUNY, Buffalo). "Spectral Properties of Plutonium: Sensitivity to 5f Occupancy," appears in *Physical Review B* **76**, 245118 (2007). DOE Basic Energy Sciences and LDRD funded the Los Alamos research.



Experimental and theoretical photoemission spectrum

Contact: John Joyce, MPA-10, jjoyce@lanl.gov

Heads UP, MPA!

MPA WSST adds environmental issues, spot awards issued

In keeping with a recent change to the Institutional WSST's charter, the MPA WSST (Worker Safety and Security Team) has added environmental concerns to its purview. Feel free to pass on concerns regarding energy consumption, recycling, environmental emissions, etc. to your local team member or to mpawsst@lanl.gov.

In recognition of exceptional response to the MPA WSST's request for action and information, the following employees will receive spot awards: Mitzi Cohn (MPA training coordinator) and Alvin Valdez, Earl Martinez and Phil Romero (OS-PT, "Gas Plant"). Congratulations!

After–hours access

In brief, employees have been finding that their after-hours building access has expired even though they are up-to-date on facility training. About a year-and-a-half ago responsibility for tracking building training and badge reader access was split between different teams and directorates.

Another important point is that the badge reader system and the training system do not "talk" to each other. These systems were previously monitored closely by one team. Now they are not. The end result is that we are not getting as good of service as we used to and people are finding their access expired.

There is a beta system in test which uses the badge reader system itself (not just the training system) to send out notices about expiration, which will hopefully be implemented to eliminate this issue.

In the meantime, employees needing after-hours access should either contact the STO Training Team (665-9430) to determine when access expires or fill out a facility access service request on the STO-FOD Web page to be sure of gaining access.

Additionally, whenever an employee completes a web-based facility training course they should complete a facility access service request so the operator of that badge system knows to not let access expire.

Gas plant issues

Although there have been some improvements and clarifications on Gas Plant (OS-PT) issues, some issues still remain, particularly with respect to the ordering of specialty gases. Interim MPA Division Leader Alex Lacerda will discuss these issues personally with Gas Plant management to push for simplifying this process.

Please visit our website at int.lanl.gov/orgs/mpa/mpa_wsst/index, or by clicking on the link on the right side of the MPA Division Website, int.lanl.gov/orgs/mpa/index.shtml, for more information.

Heads UP, MPA! reports on environment, safety, and health, security, and facility-related news and information.

Jaime and Lashley to co-chair CalCon materials and nano-technology symposium

Marcelo Jaime (MPA-NHMFL) and Jason Lashley (MST-6) will co-chair a symposium on materials and nanotechnology at the 63rd Calorimetry Conference, CalCon 2008, to take place in July in New Jersey.

The symposium will focus on the thermal and thermodynamic properties of fundamentally interesting condensed matter systems, technologically relevant materials, and nano/microscopic assemblies.

The topics envisioned thus go beyond calorimetry and include closely related properties and physical phenomena such as magnetism, thermal expansion, thermal transport, dielectric properties, sound propagation, ground state/low temperature properties, high pressures, and quantum aspects.

Invited speakers to the symposium include M.H.W. Chan, Pennsylvania State University; S.W. Cheong, Rutgers University; H. Kageyama, Kyoto University, Japan; M. Orendac, Safarik University, Slovakia; I. Terasaki, Waseda University, Japan; J. Wosnitza, Hochfeld-Magnetlabor Dresden, Germany; and Vivien Zapf, MPA-NHMFL.

The Calorimetry Conference brings together experts from around the world annually in the United States or Canada since 1954.

A strong and diverse technical/scientific program is planned that includes all aspects of calorimetry and thermal analysis, utilized to gain a deeper understanding of fundamental and technology relevant thermal processes in condensed matter physics, organic and inorganic chemistry, metallurgy, ceramics and earth science, pharmaceutical, biological and medicinal sciences, polymer science, nanotechnology, catalysis, kinetics and applied sciences.

Contact: Marcelo Jaime, MPA-NHMFL, mjaime@lanl.gov

(From the desk continued)

Congratulations to all contributors to the AMSC wire and cable development projects over the years.

MPA-WSST: working with you on safety and security

Please keep engaging with the Division's WSST team members. Any team member would be happy discussing and working with you on any safety issues. MPA-WSST team members are Chris Sheehan (chair), MPA-STC; Eric Bauer, MPA-10; Roger Lujan, MPA 11; Clay Macomber, MPA-MC; Chuck Mielke, MPA NHMFL; Darrell Roybal, MPA-NHMFL; and Darrick Williams, MPA-CINT. For information about MPA-WSST please visit int.lanl.gov/orgs/mpa/mpa_wsst/.

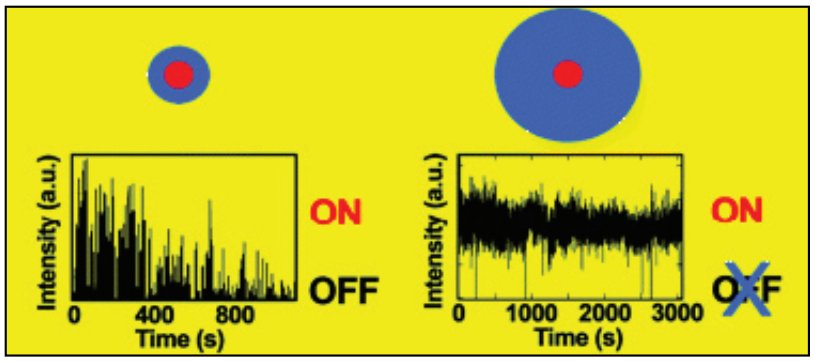
—Interim MPA Division Leader, Alex Lacerda

"Giant" quantum dots show remarkable optical properties

Semiconductor nanocrystals quantum dots are near-ideal fluorescing materials based on their unique particle-size-tunable optical properties of efficient broadband absorption and narrow-band emission. However, their optical properties are sensitive to their surface chemistry and chemical environment.

The coordinating organic ligands used to passivate the quantum surface during growth are retained following preparation and are strong contributors to bulk quantum dot optical properties, such as emission quantum yields.

Unfortunately, the ligands are labile and can become uncoordinated from the quantum dot surface and can be damaged by exposure to the light sources used for quantum dot photoexcitation. Ligand loss results in changes in quantum yields and, in the case of irreversible and complete loss, in permanent photobleaching. Quantum dots also undergo significant "blinking"(fluorescence intermittency) at the single quantum dot level.Therefore improvements in the stability of the quantum dots are needed.



Fluorescence stability time traces of single, representative quantum dots: (left) commercial Qdot655ITK, and (right) CdSe/19CdS giant quantum dots. Statistical analyses of many such time traces were used to prepare "on-time" histograms for the respective quantum dots. On-time fraction was >99% for 20% of the giant quantum dots – compared to standard commercial quantum dots for which 90% were "on" less than 35% of the time.

Chemistry Division researchers demonstrated the first all-inorganic approach to suppress blinking in these materials. They sequentially applied monolayers of inorganic shells (CdS, ZnS, or CdxZnyS alloys) around the 3-4 nm CdSe quantum dot cores to grow 15-20 nm "giant" multishell quantum dots.

The giant quantum dots have photoluminescence spectra that are shifted to longer wavelengths (lower energies) compared to the original quantum dot cores, and no photoluminescence from the shell is observed. However, absorption spectra of the giant quantum dots are dominated by the shell material.

The photo-luminescence and absorption data demonstrate that the integrity of the optically active core is uncompromised. The giant quantum dots show remarkable stability against photobleaching, changes in quantum yield, blinking, and changes in surface chemistry (see above).

These characteristics will enable applications from optoelectronics to biology that were previously hindered by quantum dot instabilities.

Researchers are Yongfen Chen, Javier Vela, Han Htoon, Joanna Casson, Donald Werder, David Bussian, Victor Klimov, and Jennifer Hollingsworth (PI) (all in C-PCS). Htoon, Klimov, and Hollingsworth hold joint appointments in the Center for Integrated Nanotechnologies.

The published research, "'Giant' multishell CdSe nanocrystal quantum dots with suppressed blinking," in Journal of the American Chemical Society 130, 5026-5027 (2008) is a research highlight (Nature 452, 916 [2008]).

The Laboratory's Laboratory-directed Research and Development progam and CINT support the research.

MPA delivers invited presentations at American Physical Society annual meeting

MPA Division was well represented at the recent American Physical Society (APS) annual meeting in New Orleans. The meeting is one of the largest technical meetings organized by the APS, attracting an average 6,000 scientists worldwide.

MPA scientists presented five invited talks: "Optical Properties of III-Mn-V Ferromagnetic Semi-conductors" by Ken Burch (MPA-CINT), "Imaging the Drift and Diffusion of Optically-Electrically-injected Spins in Semiconductors" by Scott Crooker (MPA-NHMFL), "Fermi Orbits Versus Fermi Arcs," by Neil Harrison (MPA-NHMFL), "Sliding Charge Density Wave in Manganites" by Susan Cox (MPA-NHMFL), and "The Proposed Big Light Fourth-generation Light Source at the National High Magnetic Field Laboratory" by John Singleton (MPA-NHMFL). There were also contributed talks and posters from MPA.

MPA-NHMFL article recognized as one of top 10 papers by *Journal of Physics: Condensed Matter*

An article by MPA-NHMFL researchers in collaboration with Cambridge University and Edinburgh University is recognized as one of the *Journal of Physics: Condensed Matter* Top 10 papers of 2007.

The article, "Evidence for the Charge-density-wave Nature of the Stripe Phase in Manganites," by MPA-NHMFL postdoctoral researcher Susan Cox, Jason Lashley (MST-6), E. Rosten (ISR-2), John Singleton (MPA-NHMFL), A.J. Williams (University of Edinburgh), and P.B. Littlewood (University of Cambridge) appears in *J. Phys.: Condens. Matter* **19** (2007). This is the second such recognition for MPA-NHMFL, which was included in the listing last year as well.

Contact: Susan Cox, MPA-NHMFL, scox@lanl.gov.

Materials Capability Review wraps it up

Bringing together technical staff from more than 25 groups in 10 divisions, the Materials Capability Review was held April 30-May 1 in the Study Center. The review was held in support of the Laboratory's goal of being a capabilities-based national security science laboratory.

Charged with evaluating the quality of science within the materials capability, a 11-member review committee from universities and national laboratories was presented with recent science and technological accomplishments from five theme areas representing a subset of the Laboratory's materials program—radiation-matter interactions, designed materials: synthesis, thermo-mechanical behavior, and nanomaterials, as well as current materials science at LANSCE.

Committee Chairman Tony Rollett, of Carnegie Mellon University, thanked staff members for the hard work put into the presentations and posters. Participants effectively articulated the mission relevance of their work, he said, noting the feedback delivered in last year's review.

Committee members' comments during the public out-brief featured observations on improved capability integration, the need for continuing investment in facilities, concern over retention issues, and recommendations for improvements in each theme area. Also touched upon was the importance of communicating the capability's strategic direction to all levels of staff and coupling this strategic vision with a clear, validated statement of the national need for the Laboratory's signature facility MaRIE (Matter Radiation Interactions in Extremes).

The committee's final report is expected to be issued to the PADSTE in early June. The review was hosted by the Experimental Physical Sciences Associate Director.

MPA icon contest deadline extended

MPA Division is holding a contest to create a graphical icon that represents the best of our Division's diversity, vitality, and expertise.

The MPA Council will review submissions and determine which will be the basis for the MPA icon, to be used in a variety of Division products.

The creator of the winning entry will receive a gift certificate.

Guidelines:

- Deadline for entries to kkippen@lanl.gov is June 30.
- Send your entry in its original and .pdf formats.
- When creating, keep in mind the icon will be used in a variety of formats and sizes.
- Have technical content ADC reviewed before submitting.

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www.lanl.gov/orgs/mpa/materialsmatter.shtml

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